

Born approximation for scattering of wave packets on atoms

I. Theoretical background for scattering of a wave packet on a potential field

D.V. Karlovets¹, G.L. Kotkin^{2,3}, V.G. Serbo^{2,3},

¹ Tomsk Polytechnic University, Lenina 30, 634050 Tomsk, Russia

² Novosibirsk State University, RUS-630090, Novosibirsk, Russia

³ Sobolev Institute of Mathematics, RUS-630090, Novosibirsk, Russia

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Abstract

Laser photons carrying non-zero orbital angular momentum are known and exploited during the last twenty years. Recently it has been demonstrated experimentally that such (twisted) electrons can be produced and even focused to a sub-nanometer scale. Thus, twisted electrons emerge as a new tool in atomic physics. The state of a twisted electron can be considered as a specific wave packet of plane waves. In the present paper-I we consider elastic scattering of the wave packets of fast non-relativistic particles on a potential field. We obtain simple and convenient formulae for a number of events in such a scattering. The equations derived represent, in fact, generalization of the well-known Born approximation for the case when finite sizes and inhomogeneity of the initial packet should be taken into account. To illustrate the obtained results, we consider two simple models corresponding to scattering of a Gaussian wave packet on the Gaussian potential and on the hydrogen atom. The scattering of twisted electrons on atoms will be considered in the next paper-II.

1 Introduction

Let us consider a scattering of a particle beam on a potential field. The real beam has finite sizes and nonuniform density, but usually in the standard theoretical description of the scattering process, the beam is replaced by a plane wave. Such an approach is valid for a number of problems in which distances, essential for calculation of the corresponding cross sections, are considerably smaller than the typical sizes of beam inhomogeneity. However, there are important exclusions.

Thus, at e^+e^- and ep colliders several processes were experimentally investigated and then calculated theoretically in which macroscopically large impact parameters gave an essential contribution to the cross section. These impact parameters may be much

larger than the transverse sizes of the colliding bunches. In that case, the standard calculations have to be essentially modified. It is the so called beam-size or MD-effect, discovered at the MD-detector (the VEPP-4 collider in Novosibirsk) — see review [1]. This effect is important because it leads to the essential reduction of beam particle losses at modern colliders [2]. Another important example here is the so-called pre-wave zone effect in transition radiation and diffraction radiation of electron beams [3], which is of high importance for beam diagnostic techniques in modern accelerators [4]. We should note that these phenomena are directly related to the ultra-relativistic motion of particles.

In the present paper we discuss non-relativistic elastic scattering of wave packets on the potential field in a situation when sizes of the initial packet may be comparable to the typical radius of the field action. This problem becomes especially topical due to recent experiments with the twisted electrons. These are states of the beam whose electrons have a defined value $\hbar m$ of the *orbital angular momentum (OAM) projection* on the beam propagation axis. Laser beams carrying OAM are well known in optics, [5] (for a review see [6]). Numerous applications of light with the OAM are described in the recent book [7]. History of twisted electrons is shorter. Indeed, only a few years ago, following the suggestion made in [8], several groups reported successful creation of the twisted electrons, first using the phase plates [9] and then with the computer-generated holograms [10]. Such electrons carried the energy up to 300 keV and the orbital quantum number up to $m = 200$ [11]. These vortex beams can be manipulated and focused just as the conventional electron beams, and recently remarkable focusing of a twisted electron beam to a focal spot of less than 0.12 nm in diameter was achieved [12]. It means that wave packets in the form of twisted electrons emerge as a new tool in atomic physics. One of the first atomic processes with twisted electrons – the radiative capture of twisted electrons by bare ions with the emission of a photon – was recently studied in the theoretical paper [13].

We would like to emphasize that while the use of the wave-packets instead of plane waves may be usually avoided in the standard approach (see e.g. Chapt. 4.5 in [14]), this seems to be no longer the case for scattering problems with the twisted electrons and photons. Indeed, the use of the pure Bessel (non-normalizable) states was shown to be inconsistent with the conservation law of the OAM in a $2 \rightarrow 2$ scattering, and only the formalism of the well-normalized wave packets removes this difficulty [15].

The next important theoretical problem is to study the elastic scattering of twisted electrons on atoms and atomic structures. The first theoretical investigations in this field [16, 17, 18] concentrated on some important features of such processes but do not address the generic issue: how to calculate the number of events depending on the limited sizes of the incident beam. To approach this goal, we derive a simple and convenient expression for the number of events, which generalizes the well-known Born approximation for the case when the initial beam is a wave packet, but not a plane wave. New and important feature of this problem is the fact that the observed number of events depends on the impact parameter \mathbf{b} between the potential centre and the packet axis. We also consider a case when the wave packet is scattered on the randomly distributed potential centres. From the experimental point of view, this case is the simplest one. For such a set-up we obtain a simple and transparent expression for the cross section averaged over impact parameters.

To illustrate the general formulae obtained, we consider in the present paper-I two simple models:

- 1) Scattering of the Gaussian wave packet on the Gaussian potential;
- 2) Scattering of the Gaussian wave packet on the hydrogen atom.

The detailed analysis of the angular distribution of final particles is given. Special attention is paid to the dependence of this distribution on the impact parameter of the potential centre with respect to the packet axis. It should be noted that the models being discussed have an advantage of simplicity, that is why some new features in scattering of the wave packets we study first with these models and only after that we proceed with more realistic models of the twisted electrons' wave packets.

More interesting and more sophisticated scattering of the twisted electrons on atoms will be considered in the next paper-II.

The structure of the paper-I is the following. In the next section we remind the standard Born approximation including well-known formulae for the scattering on the Gaussian potential and on the hydrogen atom. In Sect. 3 we derive the basic formulae for scattering of a wave packet on a potential field, in Sect. 4 we specify the general approach for the case of the Gaussian wave packet and illustrate this case by detailed consideration of two above mentioned models. Some conclusion is given in Sect. 5.

For definiteness, we consider below the central fields $U(r)$ having in mind that the presented method can be applied for non-central fields $U(\mathbf{r})$ as well.

To simplify formulae, we use units with the Plank constant $\hbar = 1$.

2 Standard Born approximation

2.1 Number of events in the standard Born approximation

Let us consider the scattering of a packet of non-relativistic particles (electrons, for definiteness) off a potential field $U(r)$ whose centre is located at the coordinate origin. Let the typical radius of this field's action be of the order of a . If the initial and scattered electrons have momenta \mathbf{p}_i and \mathbf{p}_f , then the S -matrix element $\langle f|S|i \rangle$ for the transition between plane waves $|i\rangle = |\mathbf{p}_i\rangle$ and $|f\rangle = |\mathbf{p}_f\rangle$ is expressed via the scattering amplitude $f(\varepsilon_i, \theta, \varphi)$ as follows:

$$\langle f|S|i \rangle = (2\pi)^2 i \delta(\varepsilon_i - \varepsilon_f) \frac{f(\varepsilon_i, \theta, \varphi)}{m_e}, \quad \varepsilon_i = \frac{\mathbf{p}_i^2}{2m_e}, \quad \varepsilon_f = \frac{\mathbf{p}_f^2}{2m_e}, \quad (1)$$

where θ and φ are the polar and azimuthal scattering angles and m_e is the electron mass. The standard differential cross section of the process equals

$$\frac{d\sigma_{st}}{d\Omega} = |f(\varepsilon_i, \theta, \varphi)|^2, \quad (2)$$

where $d\Omega$ is the solid angle element. The scattering amplitude in the first Born approximation is related to the Fourier transform of the potential field (see, for example, §126 in the text-book [19]):

$$f(\mathbf{q}) = -\frac{m_e}{2\pi} \int U(r) e^{-i\mathbf{q}\cdot\mathbf{r}} d^3r, \quad \mathbf{q} = \mathbf{p}_f - \mathbf{p}_i. \quad (3)$$

In the standard approach there is an implicit assumption that the particle bunch is wide and long and almost uniform on distances of the order of a , i.e. the bunch density

in the region of active forces is $n(\mathbf{r}, t) \approx n(\mathbf{0}, t)$, and velocities of all electrons are almost equal to each other and directed along the axis z , therefore,

$$\mathbf{p}_i = m_e \mathbf{v}_i = (0, 0, p_i).$$

In such a case the number of particles $d\nu$ scattered over the time dt is determined by a product of the differential cross section $d\sigma_{\text{st}}$ and the current of particles near the coordinate origin for a given time $v_i n(\mathbf{0}, t) dt$, while the total number of the scattered particles for the whole time reads¹

$$\frac{d\nu_{\text{st}}}{d\Omega} = L \frac{d\sigma_{\text{st}}}{d\Omega} = L |f(\mathbf{q})|^2, \quad L = \int v_i n(\mathbf{0}, t) dt. \quad (4)$$

Let the initial state be the plane wave in a large volume $\mathcal{V} = \pi \mathcal{R}^2 l_z$, where \mathcal{R} is the radius and l_z is the longitudinal length of the bunch. The bunch density during the large time $\Delta t = l_z/v_i$ is almost constant and equals $n(\mathbf{r}, t) = N_e/\mathcal{V}$, therefore,

$$L = \frac{N_e}{\mathcal{V}} l_z = \frac{N_e}{\pi \mathcal{R}^2}. \quad (5)$$

Usually, the change of the transverse beam sizes during the scattering can be neglected and the bunch density depends on the time as $n(\mathbf{r}, t) = n(\mathbf{r}_\perp, z - v_i t)$. If we define *the transverse density*

$$n_{\text{tr}}(\mathbf{r}_\perp) = \int n(\mathbf{r}, t) dz, \quad (6)$$

then quantity L coincides with the transverse density at the coordinate origin,

$$L = n_{\text{tr}}(\mathbf{r}_\perp = \mathbf{0}). \quad (7)$$

Let us remind two important examples (see, for example, problems to §126 in the text-book [19]).

2.2 Gaussian potential

The Gaussian potential has the form

$$U(r) = V e^{-r^2/(2a)^2}. \quad (8)$$

If electrons are fast ($p_i a \gg 1$) and the condition $V \ll p_i/(m_e a)$ is satisfied, then the Born amplitude equals

$$f(\mathbf{q}) = f_0 e^{-(qa)^2}, \quad f_0 = -4\sqrt{\pi} m_e V a^3. \quad (9)$$

The total cross section is determined by the small angle region $\theta \lesssim 1/(p_i a)$ and reads

$$\sigma_{\text{st}} = \frac{\pi f_0^2}{2a^2 p_i^2}. \quad (10)$$

¹For colliding beams, the quantity analogous to L is called *luminosity*.

2.3 Hydrogen atom in the ground state

The scattering of fast electrons on the hydrogen atom in the ground state is directly related to the scattering on the potential field of the form (see [19], problem 2 to §36)

$$U(r) = -\frac{e^2}{r} \left(1 + \frac{r}{a}\right) e^{-2r/a}, \quad (11)$$

where e is the proton charge and $a = 1/(m_e e^2)$ is the Bohr radius. The Born approximation for fast electrons ($p_i a \gg 1$) is valid if $m_e e^2 \ll p_i$, so the scattering amplitude is equal to

$$f(\mathbf{q}) = \frac{a}{2} \left[\frac{1}{1 + (qa/2)^2} + \frac{1}{(1 + (qa/2)^2)^2} \right], \quad (12)$$

and the total cross section is

$$\sigma_{st} = \frac{7\pi}{3 p_i^2}. \quad (13)$$

3 Scattering of a wave packet on a potential field

3.1 Basic formulae

In this section we follow the approach developed in Sect. 4.1 from the paper [1]. The initial state of incoming electrons is given by the wave packet of the form

$$\int |\mathbf{k}\rangle \Phi(\mathbf{k}) \frac{d^3 k}{(2\pi)^{3/2}}, \quad (14)$$

where the packet's wave function in the momentum space $\Phi(\mathbf{k})$ is normalized by the condition

$$\int |\Phi(\mathbf{k})|^2 d^3 k = 1. \quad (15)$$

As a consequence, the probability amplitude for the transition from this initial state to the final plane-wave state $|\mathbf{p}_f\rangle$ is given by the convolution

$$A = \int \langle \mathbf{p}_f | S | \mathbf{k} \rangle \Phi(\mathbf{k}) \frac{d^3 k}{(2\pi)^{3/2}} = \sqrt{2\pi} i \int \delta(\varepsilon - \varepsilon_f) f(\mathbf{p}_f - \mathbf{k}) \Phi(\mathbf{k}) \frac{d^3 k}{m_e}, \quad \varepsilon = \frac{\mathbf{k}^2}{2m_e}, \quad (16)$$

while the number of scattered particles equals

$$d\nu = N_e A A^* \frac{d^3 p_f}{(2\pi)^3}, \quad (17)$$

where N_e is the number of electrons in the initial packet and

$$A^* = -\sqrt{2\pi} i \int \delta(\varepsilon' - \varepsilon_f) f^*(\mathbf{p}_f - \mathbf{k}') \Phi^*(\mathbf{k}') \frac{d^3 k'}{m_e}, \quad \varepsilon' = \frac{(\mathbf{k}')^2}{2m_e}. \quad (18)$$

Taking into account that $d^3 p_f = p_f^2 dp_f d\Omega$, one can perform integration over the longitudinal momenta k_z and k'_z using the δ -functions and obtain

$$\frac{d\nu}{d\Omega} = N_e \int f(\mathbf{p}_f - \mathbf{k}) \Phi(\mathbf{k}) f^*(\mathbf{p}_f - \mathbf{k}') \Phi^*(\mathbf{k}') \frac{p_f^2}{\tilde{k}_z \tilde{k}'_z} dp_f \frac{d^2 k_\perp}{2\pi} \frac{d^2 k'_\perp}{2\pi}, \quad (19)$$

where

$$\mathbf{k} = \left(\mathbf{k}_\perp, \tilde{k}_z = \sqrt{p_f^2 - k_\perp^2} \right), \quad \mathbf{k}' = \left(\mathbf{k}'_\perp, \tilde{k}'_z = \sqrt{p_f^2 - (k'_\perp)^2} \right). \quad (20)$$

On the next step we simplify this expression using several natural assumptions. We assume that the wave packets considered have an axial symmetry, therefore, their averaged transverse momentum is zero, $\langle \mathbf{k}_\perp \rangle = \mathbf{0}$, their averaged momentum is

$$\langle \mathbf{k} \rangle = \mathbf{p}_i = m_e \mathbf{v}_i = (0, 0, p_i), \quad (21)$$

but the averaged absolute value of the transverse momentum is non-zero,

$$\langle k_\perp \rangle = \varkappa_0 = p_i \tan \theta_k. \quad (22)$$

Here we introduce the angle θ_k , which is important parameter for the twisted state and usually is called *the conical or opening angle*. The packet axis can be shifted in the transverse xy plane by a distance (by an impact parameter) b . Below we often choose the x -axis just along this shift — in this case $\mathbf{b} = (b, 0, 0)$, the azimuthal angle φ coincides with the angle between vectors $(\mathbf{p}_f)_\perp$ and \mathbf{b} , and the azimuthal angle φ_k coincides with the one between vectors \mathbf{k}_\perp and \mathbf{b} .

The packet's wave function in the momentum space can be presented as a product of wave functions corresponding to the transverse and longitudinal motions:

$$\Phi(\mathbf{k}) = \Phi_{\text{tr}}(\mathbf{k}_\perp) \Phi_{\text{long}}(k_z) \quad (23)$$

with the dispersions $\Delta k_x = \Delta k_y \sim 1/\sigma_\perp$, $\Delta k_z \sim 1/\sigma_z$, where σ_\perp and σ_z are the transverse and longitudinal averaged sizes of the packet. We assume further that these dispersions are small compared to the longitudinal momentum:

$$\Delta k_x = \Delta k_y \sim 1/\sigma_\perp \ll p_i, \quad \Delta k_z \sim 1/\sigma_z \ll p_i. \quad (24)$$

From the experimental point of view, it is interesting to consider a case when the packet's length σ_z is larger than the radius of the field action a , but still small enough to provide such a situation that during the collision time $t_{\text{col}} \sim \sigma_z/v_z = m_e \sigma_z/p_i$ the wave packet does not spread essentially in the transverse plane. It means that the collision time has to be considerably smaller than the diffraction time $t_{\text{dif}} \sim \sigma_\perp/v_\perp = m_e \sigma_\perp/\varkappa_0$. Therefore, below we assume that

$$a \ll \sigma_z \ll \sigma_\perp \frac{p_i}{\varkappa_0}. \quad (25)$$

For further integration over p_f or $\tilde{k}_z = \sqrt{p_f^2 - k_\perp^2}$ we take into account the following properties of functions under the integral. The amplitude $f(\mathbf{p}_f - \mathbf{k})$ is concentrated near the value $\tilde{k}_z = (\mathbf{p}_f)_z = p_f \cos \theta$ with the dispersion $\sim 1/a$, while the function $\Phi_{\text{long}}(\tilde{k}_z)$ is concentrated near the value $\tilde{k}_z = p_i$ with the dispersion $\sim 1/\sigma_z$, which is considerably smaller than $1/a$. Finally, we take into account that the quantities \tilde{k}_z and \tilde{k}'_z depend on k_\perp and k'_\perp but the corresponding variations are small, for example,

$$|\delta \tilde{k}_z| = \left| \delta \sqrt{p_f^2 - k_\perp^2} \right| \sim \frac{\varkappa_0 \delta k_\perp}{p_i} \lesssim \frac{\varkappa_0}{\sigma_\perp p_i} \ll \frac{1}{\sigma_z} \sim \Delta k_z \quad (26)$$

due to Eq. (25). Therefore, we can take the amplitudes $f(\mathbf{p}_f - \mathbf{k})f^*(\mathbf{p}_f - \mathbf{k}')$ out of the integral over p_f in the form $f(\mathbf{p}_f - \mathbf{p}_i - \mathbf{k}_\perp)f^*(\mathbf{p}_f - \mathbf{p}_i - \mathbf{k}'_\perp)$ with \mathbf{p}_i given in Eq. (21).

The rest integral over p_f can be evaluated as follows

$$\int \Phi_{\text{long}}(\tilde{k}_z)\Phi_{\text{long}}^*(\tilde{k}'_z) \frac{p_f^2}{\tilde{k}_z \tilde{k}'_z} dp_f = \int \left| \Phi_{\text{long}}(\tilde{k}_z) \right|^2 \frac{p_f}{\tilde{k}_z} d\tilde{k}_z = \frac{1}{\cos \theta_k}. \quad (27)$$

As a result, we obtain the basic expression

$$\frac{d\nu}{d\Omega} = \frac{N_e}{\cos \theta_k} |F(\mathbf{Q})|^2, \quad F(\mathbf{Q}) = \int f(\mathbf{Q} - \mathbf{k}_\perp) \Phi_{\text{tr}}(\mathbf{k}_\perp) \frac{d^2 k_\perp}{2\pi}, \quad (28)$$

where \mathbf{Q} is given as

$$\begin{aligned} \mathbf{Q} &= \mathbf{p}_f - \mathbf{p}_i = (\mathbf{Q}_\perp, Q_z), \quad \mathbf{Q}_\perp = (\mathbf{p}_f)_\perp = p_f(\sin \theta \cos \varphi, \sin \theta \sin \varphi, 0), \\ Q_z &= p_f \cos \theta - p_i, \quad p_f = \sqrt{p_i^2 + \varkappa_0^2}. \end{aligned} \quad (29)$$

Let us stress that the formula (28) is valid only under the condition (25) — in other words, this approximation is inapplicable for too small values of σ_\perp . Besides, we would like to note the following. To obtain this formula we have used a non-monochromatic initial packet. Moreover, in the final state we integrate over the plane waves with different energies which are detected in the solid angle $d\Omega$. Our final result (28) includes the Born scattering amplitude $f(\mathbf{p}_f - \mathbf{p}_i - \mathbf{k}_\perp)$ in which the initial plane wave has the momentum $\langle \mathbf{k} \rangle + \mathbf{k}_\perp = \mathbf{p}_i + \mathbf{k}_\perp$, while the final plane wave has the momentum \mathbf{p}_f with $|\mathbf{p}_f| = \sqrt{p_i^2 + \langle k_\perp \rangle^2} = \sqrt{p_i^2 + \varkappa_0^2}$.

Below another representation for the integral $F(\mathbf{Q})$ will be useful. It can be obtained if we substitute the evident form of the scattering amplitude from (3) into Eq. (28):

$$F(\mathbf{Q}) = -\frac{m_e}{2\pi} \int U(r) \Psi_{\text{tr}}(\mathbf{r}_\perp) e^{-i\mathbf{Q}\mathbf{r}} d^3 r, \quad (30)$$

where

$$\Psi_{\text{tr}}(\mathbf{r}_\perp) = \int \Phi_{\text{tr}}(\mathbf{k}_\perp) e^{i\mathbf{k}_\perp \mathbf{r}_\perp} \frac{d^2 k_\perp}{2\pi}. \quad (31)$$

Let us remind that in the standard approach the angular distribution of scattered particles is determined by the scattering amplitude $f(\mathbf{q})$ proportional to the Fourier-transform of the potential field $U(r)$ (see Eq. (3)). The same role for the scattering of the wave packet plays the quantity $F(\mathbf{Q})$, which is the Fourier-transform of the product of functions $U(r) \Psi_{\text{tr}}(\mathbf{r}_\perp)$ (see Eq. (30)). From here one can deduce several qualitative conclusions related to the angular distribution of the scattered electrons (see Subsection 4.1 below).

3.2 Averaging over impact parameters

Let the potential centres be randomly distributed inside a large disk of the radius $\mathcal{R} \gg a, \sigma_\perp$. In this case the averaged cross section $d\bar{\sigma}$ is obtained after the integrating the number of events over all the impact parameters \mathbf{b} and dividing the result obtained by the total number of particles in the packet:

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{1}{N_e} \int \frac{d\nu}{d\Omega} d^2 b, \quad (32)$$

where $d\nu/d\Omega$ is given by Eq. (28).

If the packet axis is shifted in the transverse plane by a distance \mathbf{b} from the potential centre, the corresponding wave function in the momentum representation can be written as

$$\Phi_{\text{tr}}(\mathbf{k}_\perp) = a(\mathbf{k}_\perp) e^{-i\mathbf{k}_\perp \cdot \mathbf{b}}, \quad (33)$$

where the function $a(\mathbf{k}_\perp)$ corresponds to a non-shifted packet. Therefore, the averaged cross section is proportional to the integral

$$I_{\text{av}} = \int F(\mathbf{Q}) F^*(\mathbf{Q}) d^2 b, \quad (34)$$

where

$$F(\mathbf{Q}) = \int f(\mathbf{Q} - \mathbf{k}_\perp) a(\mathbf{k}_\perp) e^{-i\mathbf{k}_\perp \cdot \mathbf{b}} \frac{d^2 k_\perp}{2\pi}, \quad (35)$$

$$F^*(\mathbf{Q}) = \int f^*(\mathbf{Q} - \mathbf{k}'_\perp) a^*(\mathbf{k}'_\perp) e^{i\mathbf{k}'_\perp \cdot \mathbf{b}} \frac{d^2 k'_\perp}{2\pi}. \quad (36)$$

After a trivial integration over \mathbf{b} and \mathbf{k}'_\perp , we obtain

$$I_{\text{av}} = \int |f(\mathbf{Q} - \mathbf{k}_\perp)|^2 |\Phi_{\text{tr}}(\mathbf{k}_\perp)|^2 d^2 k_\perp, \quad (37)$$

and, therefore,

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{1}{\cos \theta_k} \int |f(\mathbf{Q} - \mathbf{k}_\perp)|^2 dW(\mathbf{k}_\perp), \quad dW(\mathbf{k}_\perp) = |\Phi_{\text{tr}}(\mathbf{k}_\perp)|^2 d^2 k_\perp. \quad (38)$$

This expression can be interpreted as averaging of the standard Born cross section $d\sigma_{\text{st}}/d\Omega = |f(\mathbf{Q} - \mathbf{k}_\perp)|^2$ with the shifted momentum transfer $\mathbf{q} \rightarrow \mathbf{Q} - \mathbf{k}_\perp$ over probability $dW(\mathbf{k}_\perp)$ to have such a shift in the initial wave packet.

4 Gaussian wave packet

In this section we discuss the general properties of the Gaussian wave packets and derive the basic formulas for models mentioned in the Introduction. The obtained equations will be used for calculation of specific features of these models.

4.1 General properties

Let the initial beam be the Gaussian wave packet whose transverse wave function in the momentum representation is

$$\Phi_{\text{tr}}(\mathbf{k}_\perp) = \frac{e^{-(\mathbf{k}_\perp \sigma_\perp)^2 - i\mathbf{k}_\perp \cdot \mathbf{b}}}{\sqrt{\pi/(2\sigma_\perp^2)}}. \quad (39)$$

Therefore, the dispersion $\Delta k_x = \Delta k_y = 1/(2\sigma_\perp)$ and

$$\langle \mathbf{k}_\perp \rangle = 0, \quad \langle k_\perp \rangle = \varkappa_0 = \frac{\sqrt{\pi}}{2\sqrt{2}\sigma_\perp} \approx \frac{0.63}{\sigma_\perp}. \quad (40)$$

Taking into account inequality (24) and the relation $\varkappa_0 = p_i \tan \theta_k$, we can put below $\theta_k = 0$ for the Gaussian wave packet. The coordinate wave function reads

$$\Psi_{\text{tr}}(\mathbf{r}_\perp, t) = \int \Phi_{\text{tr}}(\mathbf{k}_\perp) e^{i[\mathbf{k}_\perp \cdot \mathbf{r}_\perp - \mathbf{k}_\perp^2 t / (2m_e)]} \frac{d^2 k_\perp}{2\pi} \quad (41)$$

and the transverse density equals

$$n_{\text{tr}}(\mathbf{r}_\perp, t) = N_e |\Psi_{\text{tr}}(\mathbf{r}_\perp, t)|^2 = \frac{N_e}{2\pi\sigma_\perp^2(t)} e^{-(\mathbf{r}_\perp - \mathbf{b})^2 / [2\sigma_\perp^2(t)]}. \quad (42)$$

For such a packet $\langle \mathbf{r}_\perp \rangle = \mathbf{b}$ and the dispersion

$$\Delta x = \Delta y = \sigma_\perp(t) = \sqrt{\sigma_\perp^2 + \left(\frac{t}{2\sigma_\perp m_e}\right)^2}. \quad (43)$$

We use the approximation (25), which implies that during the collision time the transverse dispersion $\sigma_\perp(t)$ almost does not differ from σ_\perp . In this case, the function

$$\Psi_{\text{tr}}(\mathbf{r}_\perp, t) \approx \Psi_{\text{tr}}(\mathbf{r}_\perp) = \int \Phi_{\text{tr}}(\mathbf{k}_\perp) e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} \frac{d^2 k_\perp}{2\pi} \quad (44)$$

and the quantity L from (7) (at $b = 0$) becomes equal to

$$L = n_{\text{tr}}(\mathbf{0}) = N_e \left| \int \Phi_{\text{tr}}(\mathbf{k}_\perp) \frac{d^2 k_\perp}{2\pi} \right|^2 = \frac{N_e}{2\pi\sigma_\perp^2} \quad (45)$$

(compare this expression with (5)).

If the Gaussian packet is wide, $\sigma_\perp \gg a$, the behavior of the function $U(r) \Psi_{\text{tr}}(\mathbf{r}_\perp)$ in the essential region of integration in Eq. (30) is almost the same as the one of the potential field $U(r)$. In this case the function $F(\mathbf{Q})$ has almost the same behavior as the standard Born amplitude $f(\mathbf{q})$. With the decrease of σ_\perp , behavior of these two functions becomes more and more different. For example, the decrease of the function $U(r) \Psi_{\text{tr}}(\mathbf{r}_\perp)$ with the growth of r becomes sharper and, therefore, in the function $F(\mathbf{Q})$ role of the larger values of Q , compared to the standard Born amplitude $f(\mathbf{q})$, increases. As a result, *the angular distribution becomes wider compared to the standard case*.

Let us show how the standard result follows from Eq. (28). The standard case corresponds to a wide packet which has the distribution over \mathbf{k}_\perp concentrated in the narrow region near $\langle \mathbf{k}_\perp \rangle = \varkappa_0 \approx 0$. Therefore, in the amplitude $f(\mathbf{Q} - \mathbf{k}_\perp)$ we can put $\mathbf{k}_\perp = \mathbf{0}$ and take this amplitude out of the integral over \mathbf{k}_\perp in the Eq. (28). After that this equation becomes of the form

$$\frac{d\nu}{d\Omega} = |f(\mathbf{q})|^2 N_e \left| \int \Phi_{\text{tr}}(\mathbf{k}_\perp) \frac{d^2 k_\perp}{2\pi} \right|^2, \quad (46)$$

which coincides with the standard result (4) for the number of the scattered particles if we take into account the relation (45).

Analogously, the averaged cross section for a wide wave packet coincides with the standard cross section:

$$\frac{d\bar{\sigma}}{d\Omega} = |f(\mathbf{q})|^2 \int dW(\mathbf{k}_\perp) = |f(\mathbf{q})|^2 = \frac{d\sigma_{\text{st}}}{d\Omega} \quad \text{at } \sigma_\perp \gg a. \quad (47)$$

4.2 Model 1 – scattering of the Gaussian wave packet on the Gaussian potential

For the potential field of the Gaussian form (8), the integral $F(\mathbf{Q})$ in Eq. (28) is calculated analytically

$$F(\mathbf{Q}) = B \frac{e^{(Q_\perp a)^2/(1+\sigma_\perp^2/a^2)}}{1 + a^2/\sigma_\perp^2} \frac{f(\mathbf{Q})}{\sqrt{2\pi}\sigma_\perp} e^{-i\beta}, \quad Q_\perp = p_i \sin \theta, \quad (48)$$

where

$$B = e^{-b^2/[4(\sigma_\perp^2+a^2)]}, \quad \beta = \frac{\mathbf{Q}_\perp \mathbf{b}}{1 + \sigma_\perp^2/a^2}. \quad (49)$$

The final results for the number of events and for the averaged cross section have simple analytical forms:

$$\frac{d\nu}{d\Omega} = B^2 \frac{e^{2(Q_\perp a)^2/(1+\sigma_\perp^2/a^2)}}{(1 + a^2/\sigma_\perp^2)^2} \frac{d\nu_{st}}{d\Omega}, \quad \frac{d\nu_{st}}{d\Omega} = L \frac{d\sigma_{st}}{d\Omega}, \quad L = \frac{N_e}{2\pi\sigma_\perp^2}, \quad (50)$$

$$\frac{d\bar{\sigma}}{d\Omega} = \frac{e^{2(Q_\perp a)^2/(1+\sigma_\perp^2/a^2)}}{(1 + a^2/\sigma_\perp^2)} \frac{d\sigma_{st}}{d\Omega}. \quad (51)$$

It is easy to see from this expression that for a wide beam (at $\sigma_\perp \gg a, b$) we get the standard results.

4.3 Models 2 – scattering of the Gaussian wave packet on the hydrogen atom in the ground state

The potential field of the hydrogen atom in the ground state is given by Eq. (11). In this case the integral $F(\mathbf{Q})$ in Eq. (28) can be calculated using the substitution

$$f(\mathbf{Q} - \mathbf{k}_\perp) = f_0 \left(\frac{1}{z} + \frac{1}{z^2} \right) = f_0 \int_0^\infty (1+x) e^{-xz} dx, \quad z = 1 + \frac{1}{4}(\mathbf{Q} - \mathbf{k}_\perp)^2 a^2 \quad (52)$$

and further simple integration over \mathbf{k}_\perp . As a result, the differential number of events is expressed via one-fold integral over the variable x :

$$\frac{d\nu}{d\Omega} = L f_0^2 \left| \int_0^\infty e^{-xg_0 - ig_1 b \cos \varphi - g_2 b^2} \frac{1+x}{1+x/s} dx \right|^2, \quad L = \frac{N_e}{2\pi\sigma_\perp^2}, \quad s = \frac{4\sigma_\perp^2}{a^2}, \quad (53)$$

$$g_0 = 1 + \frac{(Q_\perp a)^2}{4(1+x/s)} + \frac{(Q_z a)^2}{4}, \quad g_1 = \frac{x}{x+s} Q_\perp, \quad g_2 = \frac{1}{(x+s)a^2}. \quad (54)$$

It is easy to check that Eq. (53) does not change under the replacement $\varphi \rightarrow \pi + \varphi$. It means that the number of events is symmetric with respect to the angle $\varphi = \pi$.

In a similar way, the averaged cross section (38) can be calculated using the substitution

$$|f(\mathbf{Q} - \mathbf{k}_\perp)|^2 = f_0^2 \left(\frac{1}{z^2} + \frac{2}{z^3} + \frac{1}{z^4} \right) = f_0^2 \int_0^\infty (x + x^2 + \frac{1}{6}x^3) e^{-xz} dx \quad (55)$$

and further simple integration over \mathbf{k}_\perp , which results in the following expression

$$\frac{d\bar{\sigma}}{d\Omega} = f_0^2 \int_0^\infty e^{-xg} \frac{x + x^2 + (x^3/6)}{1 + x/(2s)} dx, \quad g = 1 + \frac{(Q_\perp a)^2}{4[1 + x/(2s)]} + \frac{(Q_z a)^2}{4}. \quad (56)$$

In the limiting case of the wide packet (at $\sigma_{\perp} \gg a, b$) we obtain

$$g_0 = g = 1 + (qa/2)^2, \quad g_1 = g_2 = 0, \quad \frac{d\nu}{d\Omega} = L f_0^2 \left(\frac{1}{g} + \frac{1}{g^2} \right)^2, \quad \frac{d\bar{\sigma}}{d\Omega} = f_0^2 \left(\frac{1}{g} + \frac{1}{g^2} \right)^2, \quad (57)$$

i. e. the standard results.

4.4 Comparison of models

In this section we compare scattering of the Gaussian packet on the Gaussian potential and on the hydrogen atom in the ground state. All figures in this subsection are calculated at $p_i a = p_f a = 10$ (for the scattering on the hydrogen atom it corresponds to the energy $\varepsilon_i = 1.36$ keV).

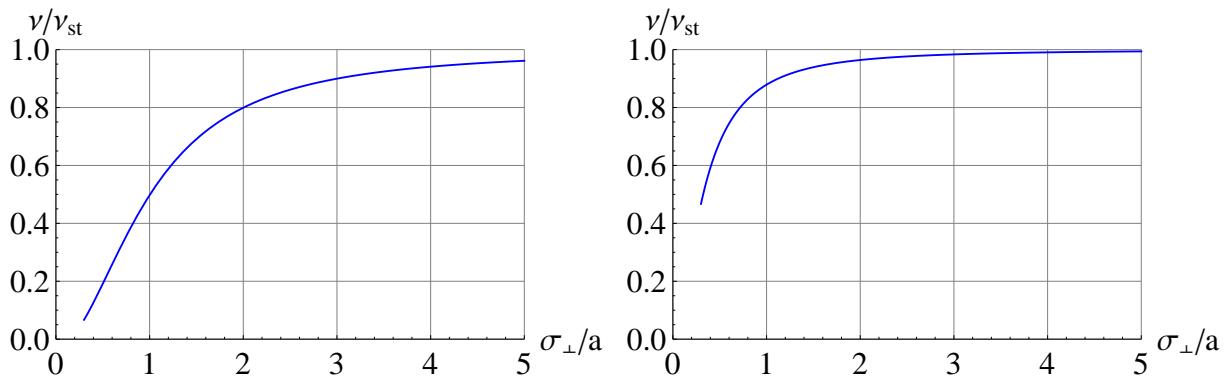


Figure 1: (*Left*) Scattering of the Gaussian packet on the Gaussian potential. Relative number of events vs. σ_{\perp}/a at $b = 0$. (*Right*) The same, but for scattering on the hydrogen atom

4.4.1 Central collision (the case $b = 0$)

Let us consider first the case of the central collision, when the impact parameter $b = 0$. What happens to the number of events ν with the decrease of the transverse bunch size σ_{\perp} ? It is clearly seen from Fig. 1 that the ratio of ν to the standard number of events ν_{st} decreases. On the contrary, the angular distribution $d\nu(\theta)/d\Omega$ or $d\bar{\sigma}(\theta)/d\Omega$ over the polar angle θ becomes wider with the decrease of σ_{\perp} (just as we expected – see Sect. 4.1). This feature is illustrated by Fig. 2, which presents the relative angular distributions

$$\frac{d\bar{\sigma}(\theta)/d\Omega}{d\bar{\sigma}(0)/d\Omega} \quad (58)$$

for $\sigma_{\perp}/a = \infty, 1, 0.3$. The physical picture is that with the decrease of σ_{\perp} , the density of the particle current increases in the vicinity of the potential centre and more particles is scattered at larger angles, but probability of such scattering becomes less (the analytical expression (51) supports such an interpretation).

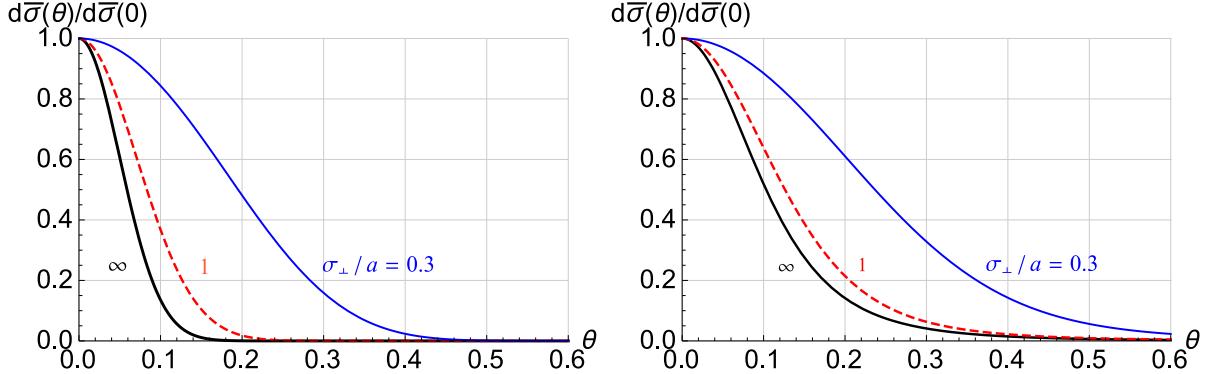


Figure 2: (Left) Scattering of the Gaussian packet on the Gaussian potential. Relative differential averaged cross section $[d\bar{\sigma}(\theta)/d\Omega]/[d\bar{\sigma}(0)/d\Omega]$ at different values of $\sigma_{\perp}/a = 0.3, 1, \infty$ (from top to below). (Right) The same, but for scattering on the hydrogen atom

4.4.2 The case $b \neq 0$

The number of events drops quickly with the increase of impact parameter b . It is clearly seen for the model 1 where all the dependance on b is determined by the function $B^2(b)$ (see Eqs. (49) and (50)). This function is presented in Fig. 3 for $\sigma_{\perp}/a = \infty, 2, 1, 0.3$. It is seen that this dependence is absent for the standard cross section (at $\sigma_{\perp} \gg a, b$). But with the decreasing σ_{\perp} , the observed cross section drops more and more quickly with the growth of b .

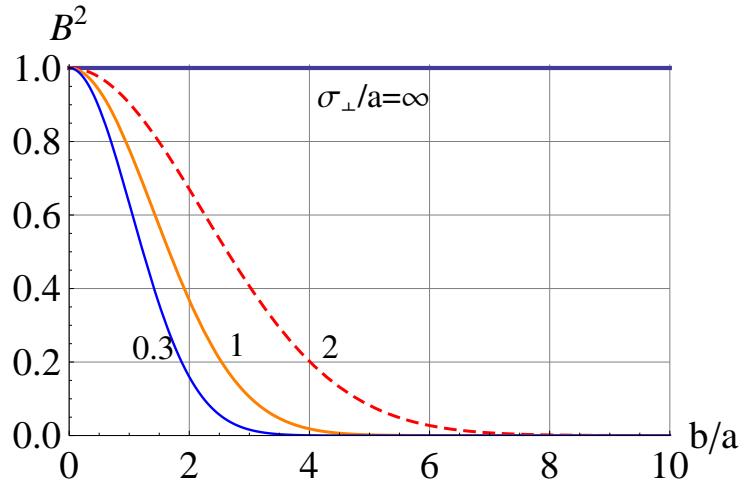


Figure 3: Scattering of the Gaussian packet on the Gaussian potential. The function B^2 vs. b/a at $\sigma_{\perp}/a = \infty, 2, 1, 0.3$ (from top to below)

From the general point of view we expect that an azimuthal asymmetry should appear in the angular distribution at $b \neq 0$. It is quite interesting to note that for the particular model 1 this general expectation is not true! Indeed, though the quantity $F(\mathbf{Q})$ (48) has the factor $e^{-i\beta}$, which does depend on the azimuthal angle between vectors \mathbf{Q}_{\perp} and \mathbf{b} , but the number of events, proportional to $|F(\mathbf{Q})|^2$, does not depend on this angle.

In contrast to the model 1, the azimuthal asymmetry appears in the model 2. For this

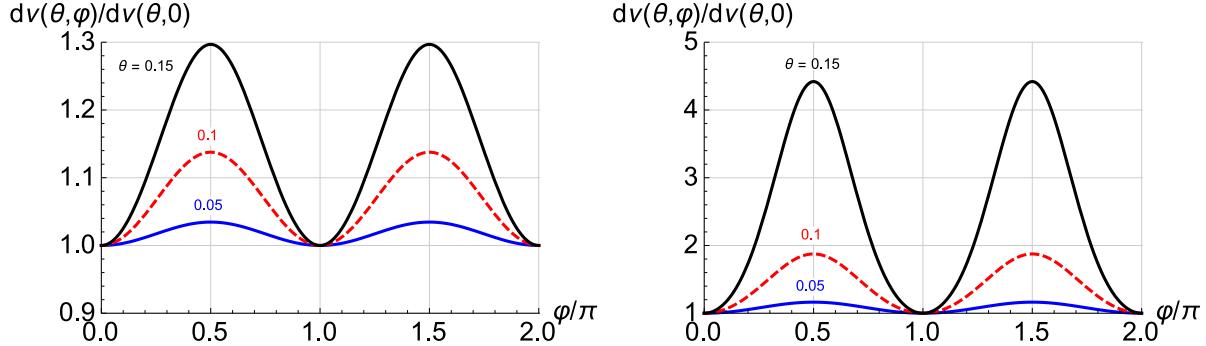


Figure 4: (*Left*) Scattering of the Gaussian packet with $\sigma_{\perp} = a$ on the hydrogen atom in the ground state. Relative differential number of events vs. azimuthal angle φ at $b = 2.5a$ and $\theta = 0.15, 0.1, 0.05$ (from top to below). (*Right*) The same, but for $b = 5a$

model at $\sigma_{\perp} = a$ we present in Fig. 4 the quantity

$$\frac{d\nu(\theta, \varphi)/d\Omega}{d\nu(\theta, 0)/d\Omega} \quad (59)$$

for different values of the polar angle $\theta = 0.05, 0.1, 0.15$. The left panel corresponds to the impact parameter $b = 2.5a$, while the right panel — to the larger impact parameter, $b = 5a$. It is seen that the discussed ratio of cross sections increases considerably at the angles of $\varphi = \pi/2$ and $\varphi = 3\pi/2$ with the growth of the impact parameter.

5 Summary

We derived a simple and convenient expression for the number of events, which generalizes the well-known Born approximation for the case when the initial beam is a well-normalized wave packet, but not a plane wave. Then we considered a couple of simple models corresponding to scattering of the Gaussian wave packet on the Gaussian potential and on the hydrogen atom.

The detailed analysis has been performed of how the total number of events and its angular distributions depend on the limited sizes of the incident beam and on the impact parameters between the potential centre and the packet's axis. In particular, we have found that the angular distributions of the effective cross section broaden with the decrease of the packet's width — this behaviour is somewhat similar to the pre-wave zone effect in transition radiation, see Ref.[3]. The non-zero impact parameter of the wave packet was shown to lead to azimuthal asymmetry, but, somewhat unexpectedly, this natural effect is absent in the model of the Gaussian potential.

In the next paper we will apply the obtained formulae for scattering of the limited twisted packets on atoms.

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